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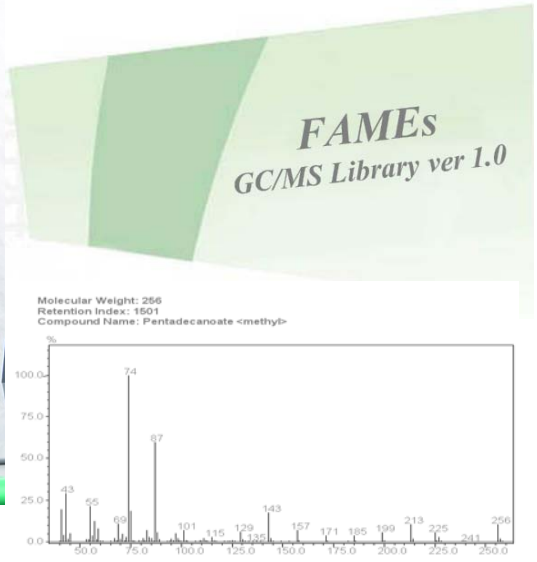
Academic Spin-off with the University of Messina

FAMEs GC/MS Library

Fatty Acid Methyl Esters Library ver 1.0
For Shimadzu GCMS-QP2010 Series

Powerful Backup to Identification of Fatty Acid Methyl Esters



240 Compounds:

Mass Spectra and Retention Indices Contained in Special Library

Through Linking with Similarity Search with Retention Index supported by GCMSsolution

Highly Reliable and Efficient Identification is Achieved for Fatty Acid Methyl Esters

Similarity Search with Retention Index

The retention index is calculated automatically by GCMSsolution.
Similarity search with retention index enables greater reliability of search results by matching retention indices with those of compounds contained within the mass spectral libraries.

Unequivocal Identification for Compounds with Similar Mass Spectra such as Isomers and Homologs.

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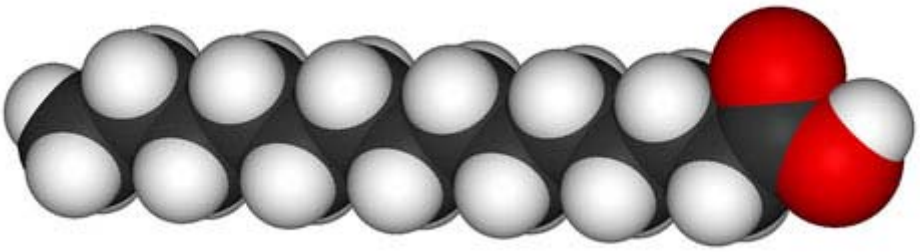
FAMEs GC-MS Library

Mass spectrometry is an analytical technique, useful to identify unknown compounds; however, to increase the power of such an instrument, large mass spectra databases are needed to match the ion fragmentation of the unknown compound.

Often dedicated libraries could be much more useful, in particular for specific fields of research (*e.g.*, industrial, academic, pharmaceutics, etc.) or samples.

Fatty acids are very important compounds since they are sample specific. They can be used as markers or their profile can be used as a fingerprint (*e.g.*, bacteria fatty acids) or to reveal fraud (*e.g.*, seed oil added to olive oil)

In GC, fatty acids are analyzed after derivatization to methyl esters; thus, a library of 240 fatty acid methyl esters (FAMEs) has been built.



The library was obtained under the conditions shown in Table 1.

Table 1. Instrument conditions

Gas Chromatograph	**GCMS-QP2010-Plus (Shimadzu)**
Automatic sampler	AOC-20i (Shimadzu)
inlet	split/splitless injector
column	Supelcowax 30 m x 0.25 mm x 0.25 µm (Supelco)
	SPB-5ms 30 m x 0.25 mm x 0.25 µm (Supelco)
carrier gas	Helium in costant linear velocity mode (35 cm/s)
Oven program temperature	50°C to 280°C (or 350°C) at 3°C/min
Mass Spectrometer	**QP2010-Plus**
Ion source temperature	220°C
Interface temperature	250°C
Scan range	50-550 u
Electron Impact (EI)	70 eV

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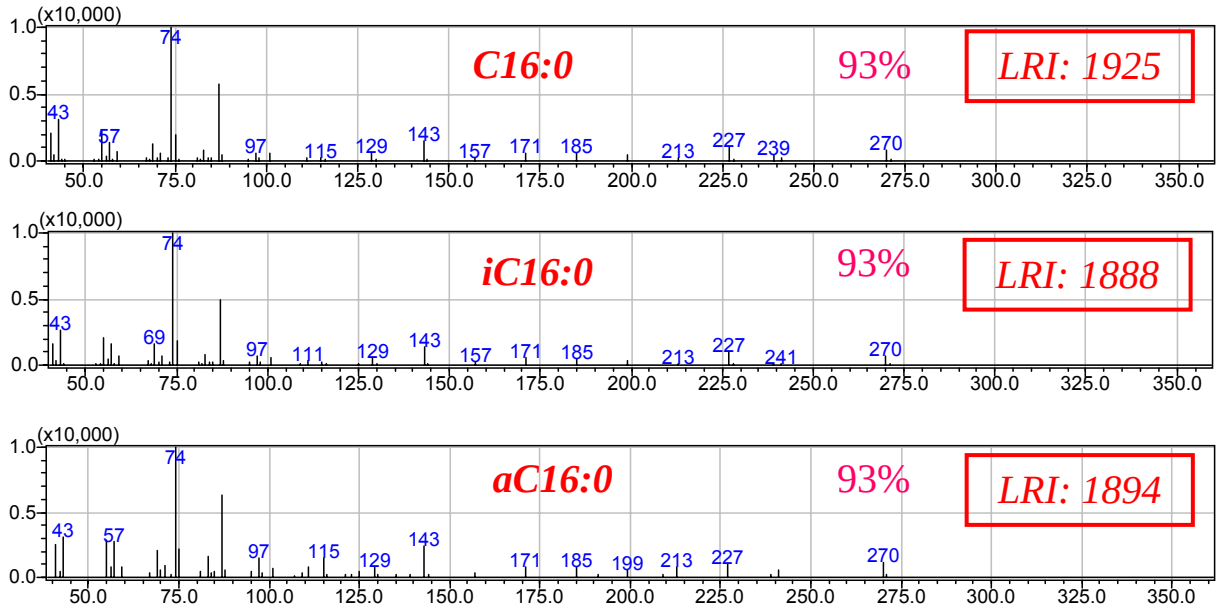
The database contains linear retention index data, registered using an alkane mixture on an apolar column and using also a FAMEs and a FAEEs (fatty acid ethyl esters) mixture on a polar one.

The library match is not enough for reliable identification of unknown compounds, since ion fragmentation patterns can be similar for several compounds.
Therefore another filter is needed!

Linear retention index (LRI) values are the most suitable choice, since they do not depend on linear velocity, column length, and temperature program.

$$100 \times \left[n + \frac{t_{R(x)} - t_{R(z)}}{t_{R(z+1)} - t_{R(x)}} \right]$$

Figure 1.Example of mass spectrum similarity of different FAMEs, which can be reliably identified only considering the LRI



Automatic search using two filters:

1- similarity

2- LRI agreement

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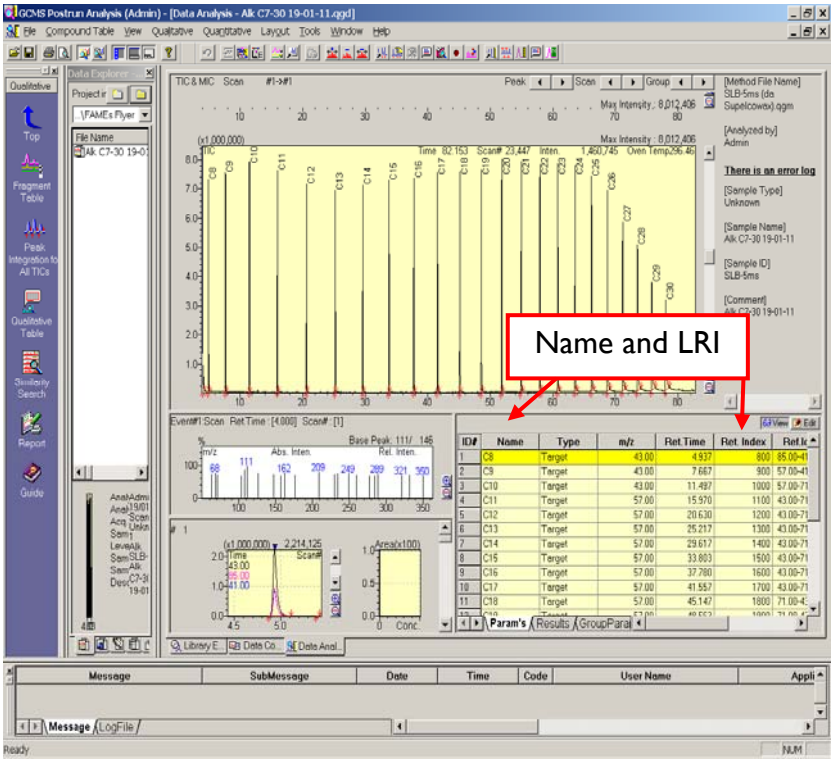
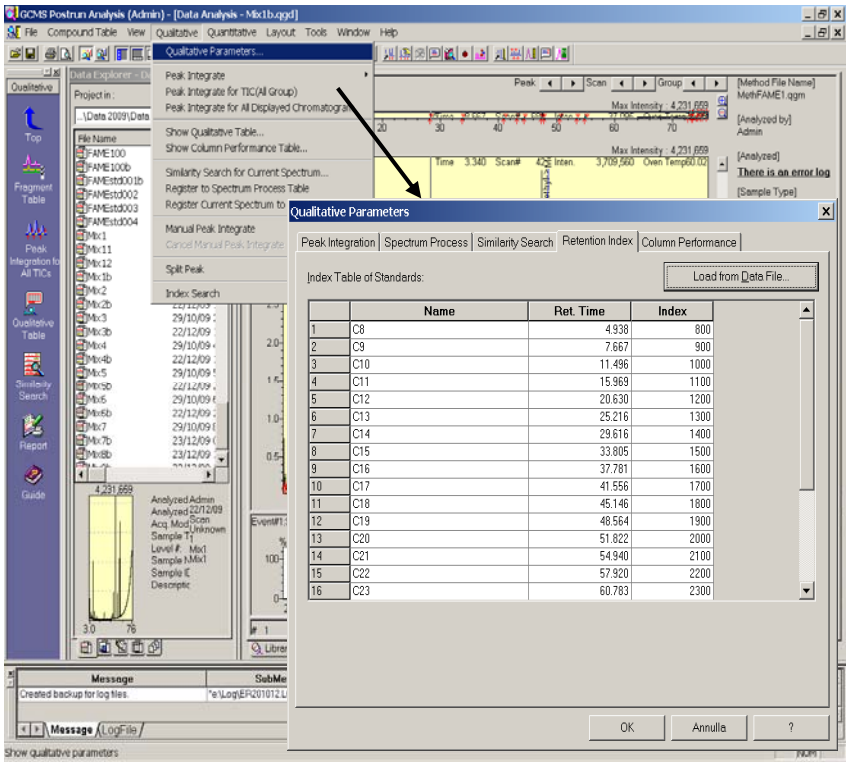
How to use the LRI filter:

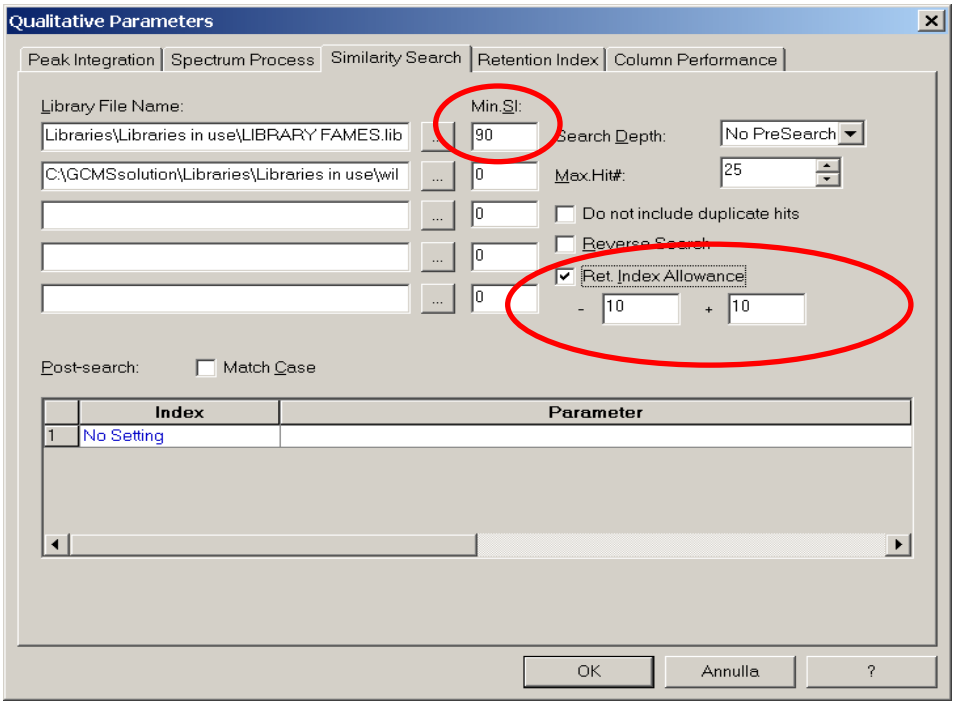
1- Inject an alkanes (FAMEs or FAEEs) mixture, register the name of each peak with the relative LRI on the compound table, and save the file.

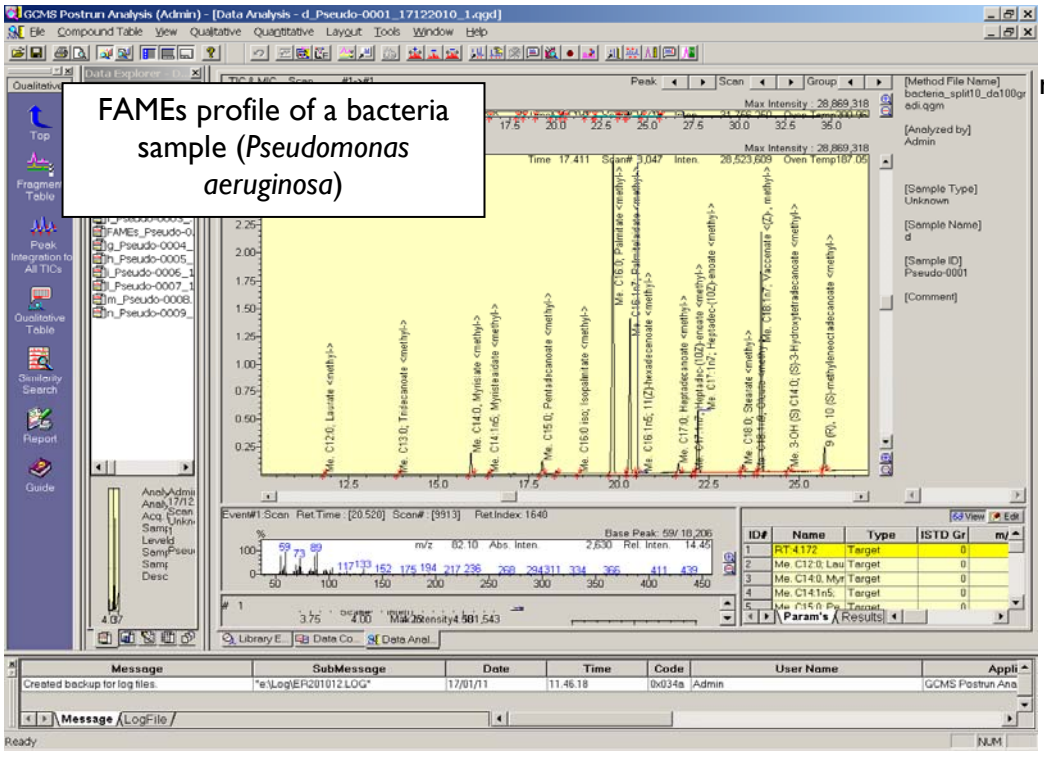




2- Inject your sample and upload the file created in point 1 in the "retention index" page of the "qualitative parameter" window

3- Set the parameters of the similarity match and LRI allowance





4- Now you are ready to identify an unknown sample!

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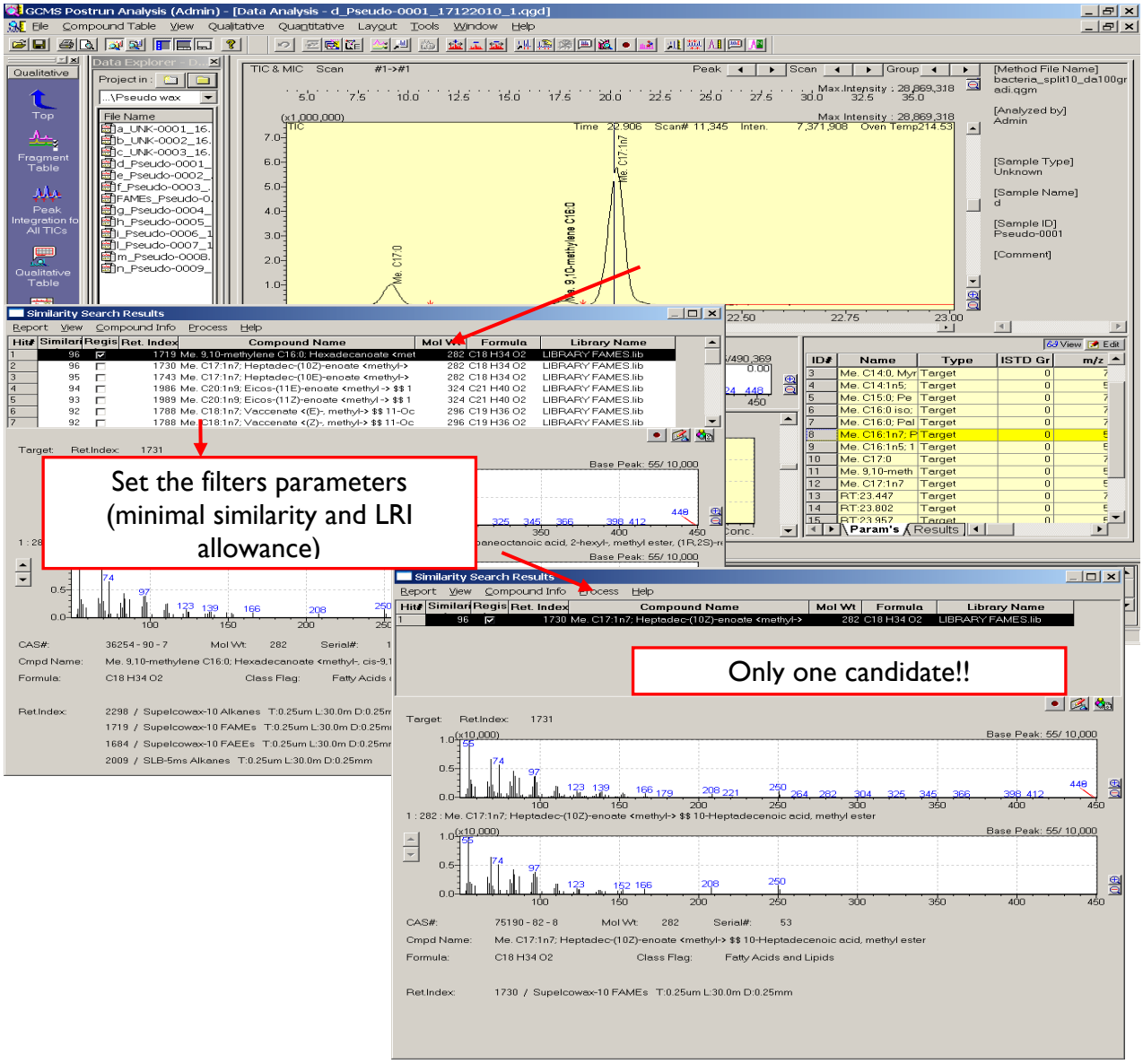

The retention index allowance windows and the tolerance range have been calculated by means of multiple injections of compounds for testing the repeatability. Due to the low solubility of n-alkanes in the polar stationary phase, FAMEs and FAEEs standard mixtures have been used to calculate LRIs on the Supelcowax-10 column. In table are reported LRI repeatability data (expressed as difference between the LRIs), calculated for a series of randomly-selected compounds.

Hit	COMMON NAME	CAS NAME	LRI FAEEs	Inj 1	Inj 2	Dif. Inj 1	Dif. Inj 2
46	Me, C11:0; Undecanoate <methyl>	Undecanoic acid, methyl ester	1058	1059	1058	-1	0
49	Me, C15:0; Pentadecanoate <methyl>	Pentadecanoic acid, methyl ester	1462	1462	1462	0	0
68	Me, C19:0; Nonadecanoate <methyl>	Nonadecanois acid, methyl ester	1867	1869	1865	-2	2

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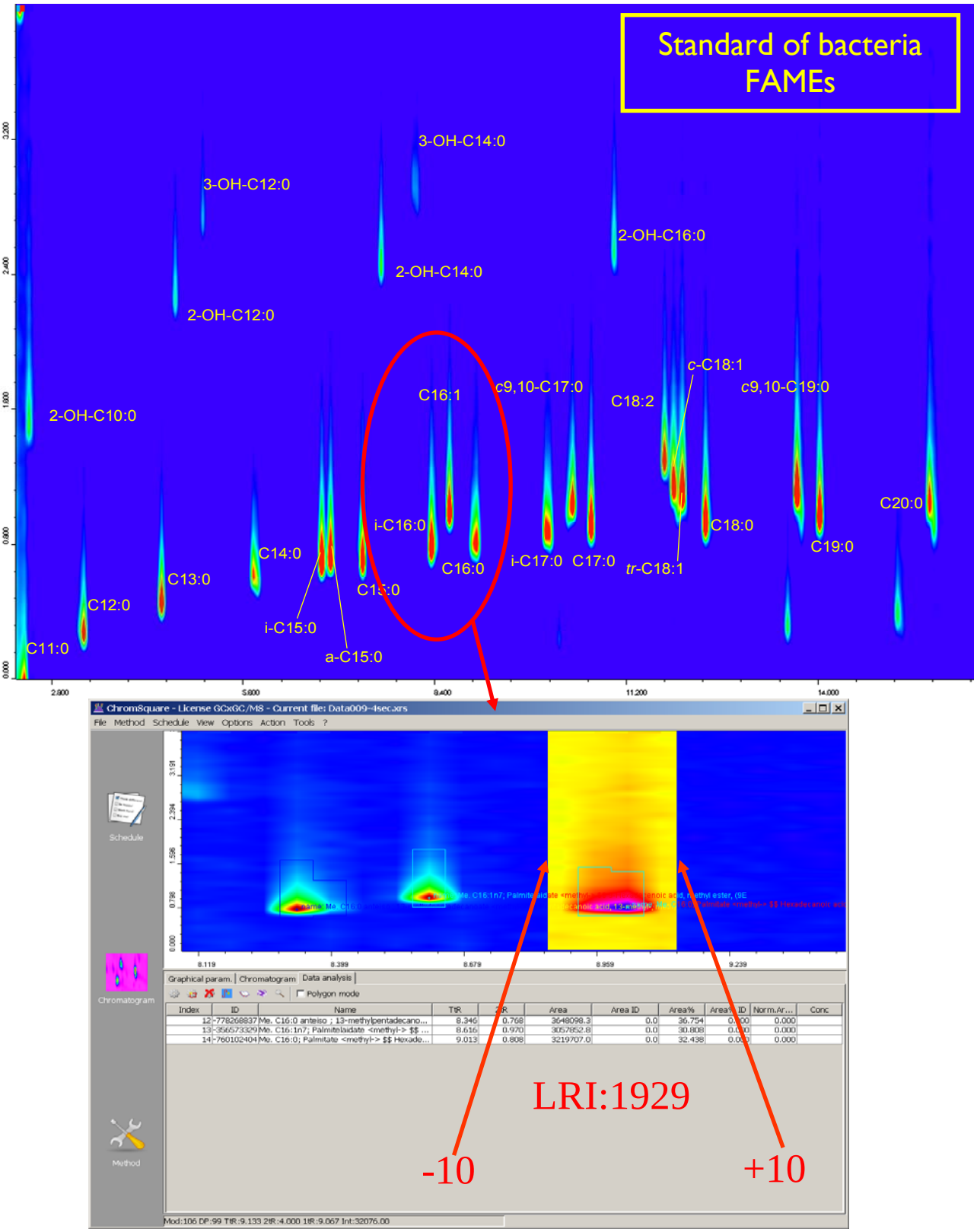
The use of the double filter is suitable also for comprehensive GC!



Chromaleont is a Society that offers solutions for the development of analytical instrumentation and dedicated software for chemical analysis and consulting in the field of Separation Science. The scope is therefore the development of new analytical methodologies for the analysis of complex mixtures by using innovative analytical instrumentation.

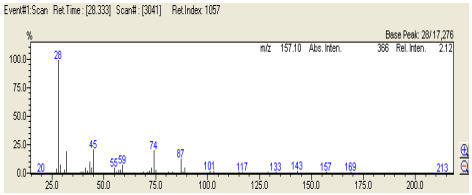
Chromaleont spin-off with the University of Messina has its office at "The Mediterranean Separation Science Foundation Research and Training Center" guest in the Dipartimento Farmaco-chimico of the School of Pharmacy of the University of Messina.

For information about Chromaleont, please visit our Web site at **www.chromaleont.it**
To contact us: **chromaleont@chromaleont.it**

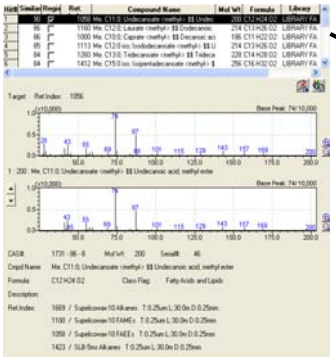
Retention Index Search - Greater Assurance and Efficiency of Identification -

Target Spectrum

Retention Index Automatic Calculation
Retention Index : 1057



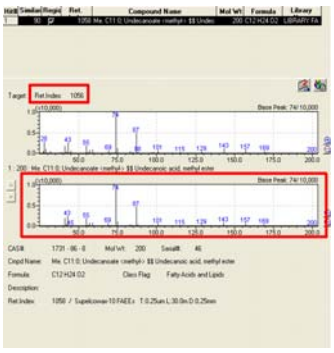
Until Now:
Similarity Search



Similarity 80 or more

Many hits, but
Identification is difficult

FAMEs GC/MS Library : Similarity Search + Retention Index Search



Similarity 80 or more
+
Retention Index calculated against FAEEs:

Tolerance Range : ± 10

Identification Is Easy!

Conventional library search, making use of solely spectral similarity, often indicates so many probable candidates for an unknown that it is hard to identify it, especially in the case that sample includes isomers and much matrix. GCMSsolution provides "similarity search with retention index", using retention indices registered in FAMEs GC/MS Library. This function makes it possible to perform more reliable and easier search even for complex samples. The results can be output as reports in electronic or hardcopy.

*FAMEs GC/MS Library can be used for GCMSsolution Ver 2.4 or higher.

Key contents

- Each record contains the mass spectrum, searchable structure, chemical information, and LRI retention data
- Records indexed by name, molecular weight, and retention time
- Highly controlled: Measured on a single instrument in controlled conditions
- Quality samples sourced from leading suppliers and manufacturers

Also available in five manufacturer formats for use with most common mass spectrometry applications: (1) NIST MS Search, (2) Agilent Chemstation, (3) PerkinElmer TurboMass, (4) ThermoFisher Spectral ID, (5) Waters MassLynx.
For more info visit the site: http://www.wiley.com